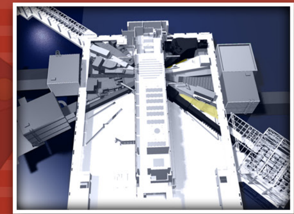
INSTRUMENT Fact Sheet

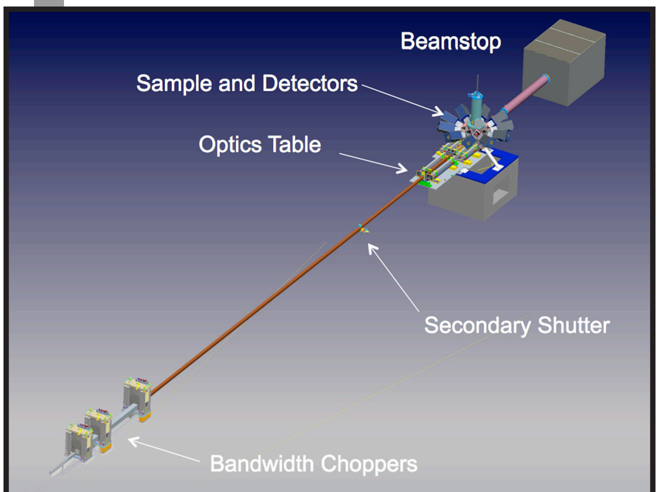


BEAM LINE 11B

SPALLATION NEUTRON SOURCE

MaNDi – Macromolecular Neutron Diffractometer

MaNDi allows the study of single crystals and is optimized for rapid data collection from large macromolecular structures. MaNDi will achieve 1.5 Å resolution from crystal volumes between 0.1 and 1.0 mm^3, with lattice repeats on the order of 150 Å. With larger crystals (>1 mm^3), it will be possible to obtain useful data in the resolution range of 2.0 to 2.5 Å for unit-cell repeats of up to 300 Å, a revolution in neutron macromolecular crystallography (NMC). Experimental duration times are to be between one and seven days, which will revolutionize NMC for applications in the fields of structural biology, enzymology, and computational chemistry.



The MaNDi detectors are designed to cover a large solid angle to record most of the neutrons scattered from a single-crystal sample, regardless of the reflection angle. This capability is accomplished through the instrument design, which places the detectors approximately spherically around the sample. The detector design follows a modular approach. A spherical detector mount will be constructed to accommodate the appropriate number of individual modules of two-dimensional, time-sensitive detectors with front face dimensions of 150 × 150 mm, leaving openings for the sample orienter/environment (top) and the incident and exiting direct neutron beam (horizontal plane). The spatial resolution of the detector is 1 mm, with a minimal sensitivity to gamma rays, hence preserving the signal-to-noise ratio of the Bragg peaks. The efficiency of this type of detector using a 1.5-mm-thick scintillator is 78% for neutrons with a wavelength of 1 Å. An increase in neutron wavelength is coupled with an increase in detection efficiency.

Precision mounting will place the 0.1-mm^3 crystals within the neutron beam, and the sample-positioning system will allow translation and rotation in x, y, and z to precisely align the sample. These operations will be remotely controlled and motor driven by a user-friendly graphical user interface.

Applications

MaNDi offers radical new opportunities for scientific studies involving the following:

- Molecular magnets, computational chemistry, and fibers
- Protein studies to provide better drug molecules for the treatment of cancer and HIV
- Studies of enzyme mechanisms to accelerate important industrial reactions
- Mechanisms used by plants to convert light into energy

Specifications

Moderator	Decoupled hydrogen
Source-to-sample distance	30 m
Sample-to-detector distance	0.45 m
Initial angular detector coverage	3 sr
Optional angular detector coverage	7 sr
Detector pixel size	6.2×10^{-6} sr (>1 mm)
Detector angles	0–180°
Wavelength bandwidth	2.16 Å
Resolution	$\Delta d/d = 0.0015$
Sample size	0.1 mm^3
Divergence	6–16 mrad

Status:
To be commissioned in 2012

For more information, contact

Instrument Scientist: Leighton Coates, coatesl@ornl.gov, 865.241.3427

http://neutrons.ornl.gov/instruments/SNS/MaNDi

May 2011

07-G00833C/gim